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"Electronic Structure and Energetics of Fullerites, Fullerides, and Fullerene Polymers"

Electronic properties of C₆₀ fullerites, various C₆₀ compounds including superconducting alkali fullerides and alkaline-earth fullerides, and polymerized C₆₀ materials, will be discussed based on the electronic structure obtained in the framework of the density functional theory. Also rich cohesive mechanisms of C₆₀ shown in various environments, i.e. van der Waals, ionic, and metallic cohesions, and even covalent bondings, will be discussed also. The C₆₀ fullerene is an atomlike building block of materials with a variety of properties which one single atom can never show. The presence of two facets on C₆₀, pentagons and hexagons, is pointed out to be very important in considering their solid-state electronic properties.